

Correlation Functions in $SU(2)$ -Invariant Resonating-Valence-Bonds Spin Liquids on Nonbipartite Lattices

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We introduce a Monte Carlo scheme based on sampling of Pfaffians to investigate Anderson's resonating-valence-bond (RVB) spin liquid wave function on the kagome and the triangular lattice. This eliminates a sign problem that prevents utilization of the valence bond basis in Monte Carlo studies for non-bipartite lattices. Studying lattice sizes of up to 600 sites, we calculate singlet-singlet and spin-spin correlations, and demonstrate how the lattice symmetry is restored within each topological sector as the system size is increased. Our findings are consistent with the expectation that the nearest neighbor RVB states describe a topological spin liquid on these non-bipartite lattices.

Introduction. It has been almost four decades since Anderson proposed[1] the quantum spin liquid state. Its undiminished appeal stems from a variety of applications from high temperature superconductivity[2] to quantum computing [3, 4]. The nature of the short ranged variant of Anderson's "resonating valence bond" (RVB) spin liquid as a topological phase became understood through a series of papers[5–7]. In particular, the invention of quantum dimer models[7] as an approximation to spin models finally lead to a lattice model exhibiting a topological RVB liquid phase[8, 24]. This however, did not immediately address the (original) question whether this exotic phase could be stabilized within the phase diagram of $SU(2)$ -invariant local spin-1/2 Hamiltonians. This was subsequently established for highly decorated lattices[9] and certain bipartite lattices [10], by finding a parent Hamiltonian for the simplest, i.e., nearest neighbor version of the prototypical RVB spin liquid wave function on such lattices. Work on quantum dimer models[8, 11–13], however, strongly suggests that nearest neighbor RVB states should be critical on bipartite lattices, as demonstrated recently[16, 17]. They should describe a \mathbb{Z}_2 -spin liquid with exponentially decaying correlations only in the nonbipartite case. While rigorously proven in the quantum dimer case, it is highly non-trivial establish this statement for the spin-1/2 RVB wave functions, due to orthogonality issues (cf, e.g., [14]). In the nonbipartite case, the nature of the correlation functions of the local spin and valence bond operator has not yet been studied systematically. This is largely due to a sign problem that will be addressed in this work. We finally mention that for the kagome case, the short-ranged RVB state studied here has been proven to be the ground state of a local parent Hamiltonian[18] (cf. also [19, 20]). The present work will provide essential evidence from correlations demonstrating that the kagome lattice RVB ground state of the Hamiltonian given in [18] is a topological (\mathbb{Z}_2) spin liquid.

Method. The standard method for calculating correlations of these wave functions on bipartite lattices is based on the observation that a general correlator between two

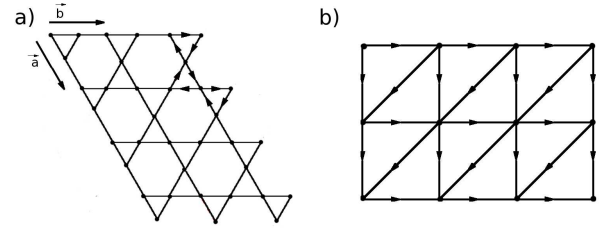


FIG. 1: a) Shape of the kagome lattice used in the calculations. The lattice consists of m unit cells in the \mathbf{a} direction and n unit cells in the \mathbf{b} direction, for a total of $3mn$ sites. Periodic boundary conditions may or may not be introduced with periods $m\mathbf{a}$ and $n\mathbf{b}$. b) The orientation used in the sign convention for the triangular lattice.

local operators \mathcal{O}_1 and \mathcal{O}_2 takes on the form

$$\frac{\langle RVB | \mathcal{O}_1 \mathcal{O}_2 | RVB \rangle}{\langle RVB | RVB \rangle} = \frac{\sum_{D, D'} \langle D | \mathcal{O}_1 \mathcal{O}_2 | D' \rangle}{\sum_{D, D'} \langle D | D' \rangle}. \quad (1)$$

Here D and D' represent dimerizations of the lattice, the sums run over all possible dimerizations, $|D\rangle$ is a nearest-neighbor valence bond (NNVB) state associated with a given dimerization and a link orientation of the lattice (defined below), and $|RVB\rangle$ is the RVB state, $|RVB\rangle = \sum_D |D\rangle$. Since every pair of dimer configurations D, D' corresponds to a configuration of non-intersecting close packed loops on the lattice, Sutherland pointed out [21] that the evaluation of such correlation functions may be reduced to the study of a classical loop gas model. This is so *provided that* the overlaps $\langle D | D' \rangle$ are strictly non-negative. Otherwise, the evaluation of these correlators through Monte Carlo methods suffers from a sign problem. Indeed, it is not difficult to show that, e.g., for the kagome lattice, for any sign convention for the states $|D\rangle$ some of the overlaps $\langle D | D' \rangle$ are always negative. It is clear that such a sign problem would never arise were we to work with an orthogonal basis. In this case only strictly positive diagonal terms appear in the denominator of the expression re-

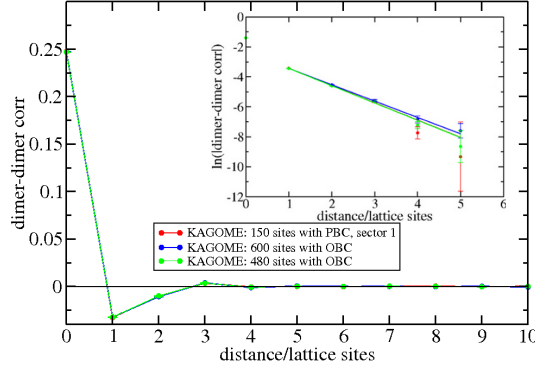


FIG. 2: The dimer-dimer correlation function shown for kagome lattices with PBCs and OBCs. Insensitivity to system size and short correlation length are evident. The PBC case has been calculated within a fixed topological sector. The inset shows a logarithmic plot including a linear fit, yielding a correlation length of 1.12(3).

placing Eq. (1). An obvious candidate for such a basis is the “Ising”-basis where local spins have definite z projection, $|RVB\rangle = \sum_I a_I |I\rangle$, and I runs over all possible Ising spin configurations. Two primary questions need to be addressed to determine whether the Ising-representation lends itself to Monte Carlo evaluation of correlations. The first is the obvious question whether for the wave function $|RVB\rangle$, the coefficients a_I in the above representation can be efficiently calculated. The second question relates to the observation that for the short-ranged RVB state $|RVB\rangle$, it turns out that only a small fraction of configurations I will lead to non-zero a_I . One may, however, ask if once an I with non-zero a_I is found, a sufficiently local update of I has a high chance of leading to a new I' with $a_{I'} \neq 0$. To proceed, we first need to express the wave function $|RVB\rangle$ in the Ising ba-

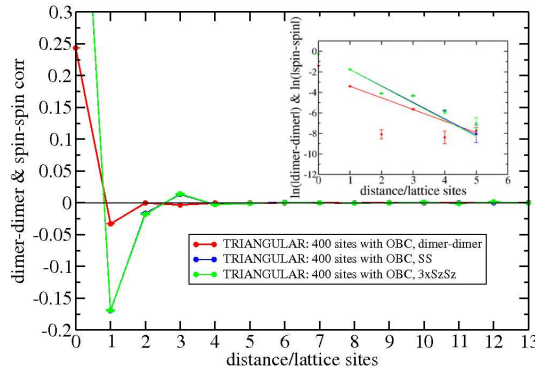


FIG. 3: The dimer-dimer and spin-spin correlation functions for a 400 sites triangular lattice with OBCs. The inset shows logarithmic plot with fits, giving a correlation length of 1.15(2) for the dimer-dimer decay. The spin-spin correlations display stronger even/odd effects at short distance. Fitting only odd distances in the spin-spin case gives a correlation length of 1.61(2).

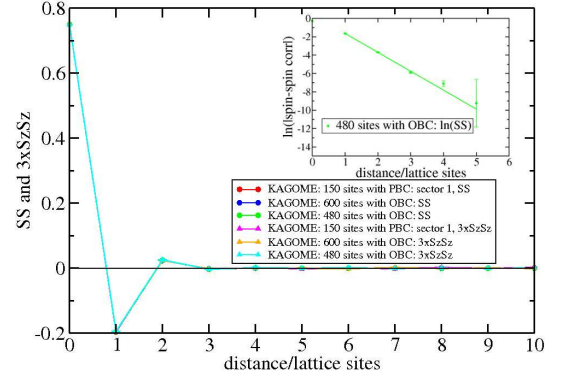


FIG. 4: The spin-spin correlation functions $\langle \vec{S}_i \vec{S}_{i+\kappa} \rangle$ and $\langle S_i^z S_{i+\kappa}^z \rangle$ for different kagome lattices (PBC and OBC). Again, the topological sector was fixed in the PBC case. The inset shows a logarithmic plot with linear fit yielding a correlation length of 2.08(2).

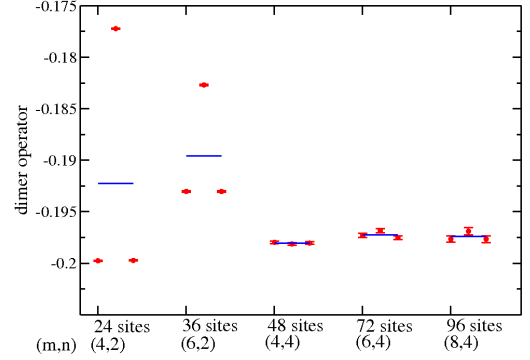


FIG. 5: The expectation value of the dimer operator for links of the three possible directions and various lattice sizes. The average for one system size is shown as horizontal bar. A topological sector has been fixed. The discrepancy between inequivalent links rapidly decreases with system size, restoring the lattice symmetry.

sis. We observe that in the Ising basis, the wave function $|RVB\rangle$ can be naturally written as a “Haffnian”[25]:

$$a_I = \text{Haff}[M_{ij}(I)] \equiv \frac{1}{2^{N/2}(\frac{N}{2}!)} \times \sum_{\lambda \in S_N} M_{\lambda_1 \lambda_2}(I) M_{\lambda_3 \lambda_4}(I) \times \cdots \times M_{\lambda_{N-1} \lambda_N}(I). \quad (2)$$

Here, M is a symmetric matrix whose indices run over the N lattice sites and which depends on the Ising configuration via $M_{ij}(I) = \Theta_{ij}(\delta_{\sigma_i, \uparrow} \delta_{\sigma_j, \downarrow} - \delta_{\sigma_i, \downarrow} \delta_{\sigma_j, \uparrow})$, where the σ_i describe the Ising configuration I . λ runs over all permutations of the N sites, and Θ_{ij} is the matrix describing the chosen orientation of the lattice. An orientation refers to a relation defined between any two nearest-neighbor lattice sites i, j , according to which either $i < j$ or $i > j$ holds. Then $\Theta_{ij} = 0$ if i, j are not nearest neighbors, $\Theta_{ij} = 1$ for $i > j$, and $\Theta_{ij} = -1$ for $i < j$.

Here we consider the orientation chosen for the kagome lattice indicated by the arrows in Fig. 1a. The formal definition of the Haffnian is related to that of the Pfaffian through omission of the sign factor $(-1)^\lambda$. While the Pfaffian and the determinant can be evaluated in polynomial time, it is not known how to do this for the other two cases. It would thus be desirable to rewrite Eq. (2) through a Pfaffian. Luckily, this is the same problem that Kasteleyn solved long ago[22], which has been a standard tool in the study of classical and quantum dimer models. In the present context, it does not seem to have enjoyed much attention. Kasteleyn evaluated the partition function of the classical dimer gas, which is exactly Eq. (2) with M_{ij} replaced by $|\Theta_{ij}|$. He found that this problem may be written as $\text{Pfaff}[\Theta_{ij}^K]$ where Θ^K is a matrix similar to Θ , but describing a different, so-called “Kasteleyn” orientation of the lattice. For planar lattice graphs, such an orientation may generally be found. A Kasteleyn orientation for the kagome lattice is given in [23]. The same method works in Eq. (2) [25]. We thus have $a_I = \text{Pfaff}[M_{ij}(I)\Theta_{ij}^K]$. We are now in a position to cast the problem of evaluating the correlation functions (1) as a *classical* statistical mechanics problem. We have:

$$\begin{aligned} \frac{\langle RVB|\mathcal{O}_i\mathcal{O}_j|RVB\rangle}{\langle RVB|RVB\rangle} &= \frac{\sum_I \sum_{I'} a_I a_{I'} \langle I'|\mathcal{O}_i\mathcal{O}_j|I\rangle}{\sum_I |a_I|^2} \\ &= \frac{\sum_I |a_I|^2 \sum_{I'} \frac{a_{I'}}{a_I} \langle I'|\mathcal{O}_i\mathcal{O}_j|I\rangle}{\sum_I |a_I|^2}. \end{aligned} \quad (3)$$

This may now be interpreted as the classical expectation value of a quantity f : $\langle f \rangle = \sum_I f_I e^{-E_I} / \sum_I e^{-E_I}$. Here, $e^{-E_I} = |a_I|^2$ and the value f_I of the quantity f in the Ising configuration I is given by $f_I = \sum_{I'} \langle I'|\mathcal{O}_i\mathcal{O}_j|I\rangle \frac{a_{I'}}{a_I}$.

We have now demonstrated that the evaluation of correlation functions can be cast in terms of a partition function, whose weights are positive and can be evaluated in polynomial time (the structure of our Pfaffian in fact allows reduction to the determinant of an $N/2 \times N/2$ matrix). Returning to our earlier caveat, we moreover found that once we have an initial Ising configuration I with $a_I \neq 0$, performing updates[25] by exchanging neighboring spins has a high chance of leading to a new configuration I' with $a_{I'} \neq 0$. The basic requirements for Monte Carlo evaluation are thus met.

Results. Simulations are now performed for different lattices sizes. For the kagome lattice, we have chosen (m, n) as defined in Fig. 1 to be (10,5) for periodic boundary conditions (PBCs) and to be (20,8) and (20,10) for open boundary conditions (OBCs), resulting in a total number of $N = 150, 480$, and 600 sites, respectively, (and in lattices with roughly unit *perpendicular* aspect ratio). For the triangular lattice, we show data belonging to a 20×20 “square” with diagonals (see Fig. 1) giving a lattice of 400 sites. In one Monte Carlo sweep through the lattice, we attempt to do a number of N exchanges

of two neighboring spins. All expectation values were calculated by making about 1,500,000 measurements on the configurations produced by the Monte Carlo process, allowing the system to equilibrate for 8000 sweeps. Autocorrelation times are generally quite low, on the order of 1.

Fig. 2 presents the connected correlation function of the “dimer” or valence bond operator $\vec{S}_i \cdot \vec{S}_{i+x}$, where i and $i+x$ are nearest neighbors, for different lattice sizes and boundary conditions. It is evident that there is a finite and very short correlation length. From the inset it is clear that the absolute values of the correlation functions follow a simple exponential law already at short distance, from which we obtain a correlation length of $\xi = 1.12(3)$. Moreover, the plot for 600 sites and OBCs coincides very well with that for 150 sites and PBCs. We note that for the case of PBCs, the method used to treat the classical dimer case[23] can again be adapted to the present situation, and yields an expression of the amplitude a_I as a superposition of four Pfaffians. Different such superpositions can be used to project onto different topological sectors of the toroidal system. While only one topological sector is shown, we have also convinced ourselves that results for different topological sectors agree within error bars. The fact that the dimer-dimer correlations are apparently insensitive to both lattice size *and* boundary conditions, already for a relatively small size of 150 sites, is consistent with the hypothesis of a gapped state. We note moreover that the decay is very reminiscent of the quantum dimer model case, where dimer-dimer correlations have been shown to decay super-exponentially, with correlations being exactly zero beyond distance 2[26]. While this is clearly not the case for the RVB state, a very short correlation length of order 1 still mimics this behavior fairly closely. The qualitative agreement between the quantum dimer model and the RVB state is thus quite striking.

Fig. 3 shows the dimer-dimer correlations for a 400 site triangular lattice, displaying similarly short ranged correlations. Subdominant corrections to the dominant exponential decay are clearly somewhat more important than for the kagome, as one would generically expect; however a correlation length close to 1.6 is still clearly visible in the inset. All linear fits are obtained from a weighted least square regression, where the weights have been chosen as the inverse squares of the error bars. Note that although the value at distance zero has not been included into any fit, even this shortest distance data point tends to follow the exponential trend very well. We point out that a sign convention for the triangular lattice exists which eliminates the sign problem of Eq. (1) [27]. Here, however, we have chosen a different convention (Fig. 1b), for which this problem persists.

We also computed spin-spin correlation functions $\langle \vec{S}_i \cdot \vec{S}_j \rangle$. Results are shown for the kagome in Fig. 4 and for the triangular lattice in Fig. 3. Spin-spin corre-

lations decay exponentially even in the critical square-lattice case[15], and by theoretical prejudice should decay exponentially for all short ranged RVB states. Moreover, even on the kagome, DMRG work has predicted a spin liquid phase with gapped spin but gapless singlet excitations[28]. This might render the singlet sector more crucial in the present context. Nonetheless, direct demonstration of the exponential decay of spin-spin correlations is not straightforward, especially in the presence of the sign problem discussed initially. Again, the short-ranged nature of the correlations is apparent in both cases. As a consistency check, both $\langle \vec{S}_i \cdot \vec{S}_j \rangle$ and $3\langle S_i^z S_j^z \rangle$ are shown, which must agree by $SU(2)$ symmetry. This symmetry is, however, not manifest in the Ising-basis we are working with. [36]

Up to now we have demonstrated that connected correlations for the RVB states on the kagome and triangular lattice are short-ranged. This does, however, by itself not guarantee the liquid property of these states. In particular, the four degenerate RVB ground states on the torus transform nontrivially under the space group of the lattice, and to demonstrate the liquid property and rule out the possibility of a valence bond solid [30], it is essential to show that the full lattice symmetry is restored in the thermodynamic limit, for each individual ground state (within each topological sector). We restrict ourselves to the kagome lattice here. In the following, we will refer to lattice links as “symmetry inequivalent” if they are not related by a symmetry of the *wave function* (even though they may be related by a symmetry of the lattice). For lattices of the shape shown in (Fig. 1a), with m, n both even, any three links along different directions will always exhaust all possible classes of inequivalent links. In Fig. 5, we plot the expectation values of the dimer operator for three such links, evaluated in one topological sector, for various “even/even” lattices. One observes that the discrepancy between inequivalent links rapidly decreases, by a factor of *at least* 60 between 24 sites and 48 sites, taking into account error bars. (The consistency between symmetry equivalent links suggests that the error is much smaller than shown, and the factor is really on the order of 100). For larger lattice size, the calculation becomes increasingly demanding, since, presumably, increasingly smaller error bars are needed to resolve the discrepancy in expectation values, while even maintaining the size of the error bars is more costly (Fig. 5). It is worth noting, though, that the average of the three expectation values for 72 and 96 sites appears to have converged, and we are thus approaching the thermodynamic limit. In all, these findings are highly consistent with the general expectation that the RVB-states describe a topological spin liquid.

Conclusion. In this work, we have studied correlation functions of nearest neighbor resonating valence bond wave functions on both the kagome and the triangular lattice, with up to 600 lattice sites. A sign problem of

earlier methods has been circumvented by using a Pfaffian representation of the wave function in the Ising basis. This allows for evaluation of correlators for both OBCs and PBCs, and, in the latter case, restriction to a single topological sector. This allowed us to present strong evidence that not only correlations decay exponentially as expected, but also that no broken lattice symmetry remains in the thermodynamic limit for the kagome lattice. For the kagome, this greatly adds to the amassed evidence that local $SU(2)$ invariant Hamiltonians stabilizing a topological spin liquid state are possible[18, 29]. Further possible applications of our method include the investigation of short-ranged RVB wave functions on other nonbipartite lattices. In particular, certain next nearest neighbor links may be introduced in standard lattice geometries such as the square lattice[31], as long as the planarity of the lattice is maintained. This makes it natural to introduce different weights for different types of valence bonds. Furthermore, our method allows for the introduction of any number of mobile (delocalized) holes and thus the study of monomer correlations and the related confinement/deconfinement issue. We are hopeful that these prospects will stimulate future work.

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Note added. After the completion of this work, Ref.[34] appeared using an approach that has been outlined in Ref.[35].

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 - [36] We note that $S^z S^z$ correlations for the kagome were also calculated very recently using a PEPS representation [29]. However, we find a direct comparison of our results not straightforward, due to the blocking procedure carried out in [29].

Supplemental material: Haffnian and Pfaffian representation of RVB state, and ergodicity

We begin with the Haffnian representation of the RVB state $|RVB\rangle = \sum_I a_I |I\rangle$. We reproduce Eq. (2) of the paper as

$$a_I = \text{Haff}[M_{ij}(I)] \equiv \frac{1}{2^{N/2}(\frac{N}{2}!)} \times \sum_{\lambda \in S_N} M_{\lambda_1 \lambda_2}(I) M_{\lambda_3 \lambda_4}(I) \times \cdots \times M_{\lambda_{N-1} \lambda_N}(I). \quad (4)$$

Independent of I , $|M_{ij}(I)|$ is just the adjacency matrix of the lattice, the only contributions come from permutations λ such that $(\lambda_{2n-1} \lambda_{2n})$ is a nearest neighbor pair, n being an integer running from 1 to half the number of lattice sites. Therefore, a contributing permutation λ corresponds to a dimerization D of the lattice into nearest neighbor pairs. The permutations corresponding to the same dimerization in this way are all related by permuting the members of the individual pairs and by

permuting pairs among each other. This over-counting is compensated by the combinatorial prefactor. The sum in Eq. (4) is thus essentially a sum over dimer configurations D . Since as function of $\sigma_{\lambda_{2n-1}}$ and $\sigma_{\lambda_{2n}}$, $M_{\lambda_{2n-1} \lambda_{2n}}(I)$ is just the wave function of a singlet occupying the link $(\lambda_{2n-1} \lambda_{2n})$, endowed with the correct sign, the contribution of a given λ to Eq. (4) is just the spin wave function associated with the dimer covering D in the RVB state.

On the other hand, the Pfaffian representation can be written as

$$a_I = \text{Pfaff}[\tilde{M}_{ij}(I)] \equiv \frac{1}{2^{N/2}(\frac{N}{2}!)} \times \sum_{\lambda \in S_N} (-1)^\lambda \Theta_{\lambda_1 \lambda_2}^K(I) \Theta_{\lambda_3 \lambda_4}^K(I) \times \cdots \times \Theta_{\lambda_{N-1} \lambda_N}^K(I) M_{\lambda_1 \lambda_2}(I) M_{\lambda_3 \lambda_4}(I) \times \cdots \times M_{\lambda_{N-1} \lambda_N}(I). \quad (5)$$

For reasons of self-containedness, we reproduce here the well-known arguments[1] that Eqs. (4) and (5) are interchangeable. This also serves to make it manifest that these arguments carry over from the original classical dimer problem to the present situation without any difficulty. We first want to see that Eqs. (4), (5) are identical within each topological sector of dimer coverings, possibly up to an overall negative sign. To this end, we use the fact that all coverings within a topological sector are mutually related by a sequence of “resonance moves”, where during a single resonance move, a set of dimers is shifted along a path of links forming a contractible (topologically trivial) loop. This interchanges occupied and unoccupied links along the loop. It is therefore sufficient to show that the additional term of Eq. (5) compared to Eq. (4) is constant under a resonance move. Without any loss of generality, we can consider permutations λ, λ' corresponding to the dimer covering before and after the resonance move, respectively, that differ by a single cyclic permutation of the values of $\lambda_1 \dots \lambda_{2k}$. Then $(-1)^\lambda = -(-1)^{\lambda'}$. Moreover, the defining property of the Kasteleyn orientation is that the number of clockwise oriented links along any contractible loop of even length, which encloses an even number of lattice sites, is odd. (To ensure this, it is sufficient that the number of clockwise oriented links is odd around any elementary plaquette of the planar lattice graph, for both even and odd plaquette perimeter). This then implies that the same cyclic permutation of indices described above also introduces an additional minus sign into the product $\Theta_{\lambda_1, \lambda_2}^K \cdots \Theta_{\lambda_{2k-1}, \lambda_{2k}}^K$. This shows that (4) and (5) are identical within a topological sector up to a sign. For open geometry, there is just one topological sector (up to “non-resonable” configurations in the triangular lattice case[2] that are of negligible weight in the RVB state), and we are done. For periodic boundary conditions (torus geometry), Eqs. (4) and (5) do in general differ by a sign that is different for different topologi-

cal sectors. However, this relative sign can be changed by further modifying Θ^K along topologically non-trivial loops[3], making it possible to render all signs identical, or, as we did, to project onto a single topological sector by taking superpositions for different such modified Θ^K .

These considerations also set us up to observe an ergodicity property that the nearest neighbor spin exchange moves employed in our Monte Carlo method have. Stated precisely, these moves are ergodic within the subset of Ising basis states that have non-zero weight for at least one nearest neighbor valence bond state (NNVB) within a given topological sector. First of all, it is obvious that nearest neighbor exchanges connect all Ising configurations belonging to a given NNVB state: Such configurations are linked by exchanges on links belonging to singlet pairs in the NNVB state. Moreover, for every dimer loop in the dimer covering associated with the NNVB state, there are Ising configurations contributing to this state that are Neel ordered along this loop.

Such Ising configurations, however, have non-zero weight not only in this particular NNVB state, but also in the NNVB state whose dimer configuration differs from the original one by a single resonance move along this particular dimer loop. Then, by induction over the minimum number of resonance moves needed to connect two dimer coverings in the same topological sector, all Ising basis states having non-zero weight in the NNVB states associated with these coverings can be connected by nearest neighbor spin exchanges.

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